wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2024 – 10:41 PM EST

PDB ID	:	4LK1
Title	:	Crystal Structure Analysis of the E.coli holoenzyme
Authors	:	Bae, B.; Darst, S.A.
Deposited on	:	2013-07-05
Resolution	:	3.84 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

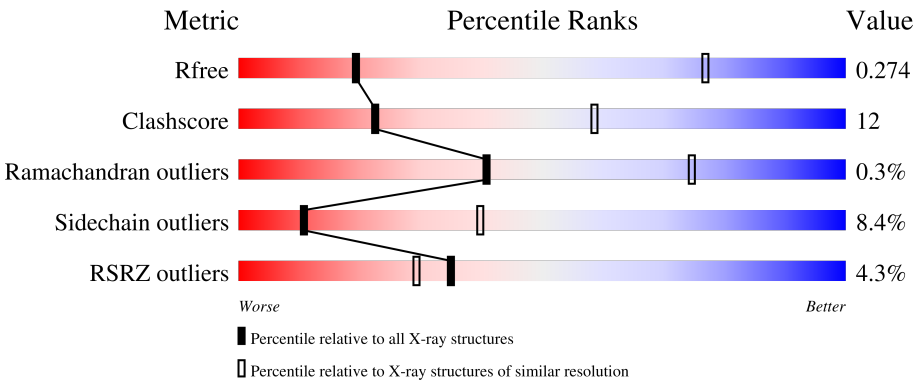
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.84 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1242 (4.08-3.60)
Clashscore	141614	1004 (4.04-3.64)
Ramachandran outliers	138981	1003 (4.06-3.62)
Sidechain outliers	138945	1266 (4.08-3.60)
RSRZ outliers	127900	1149 (4.08-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	239	% 64% 28% • 6%
1	B	239	6% 59% 30% • 8%
1	G	239	3% 64% 28% • 5%
1	H	239	8% 57% 31% • 9%
2	C	1342	2% 68% 29% •

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Mol	Chain	Length	Quality of chain
2	I	1342	4% 69% 29%
3	D	1407	2% 55% 25% 17%
3	J	1407	7% 62% 29% 5%
4	E	91	68% 26%
4	K	91	62% 23% 13%
5	F	613	6% 61% 25% 12%
5	L	613	5% 61% 25% 12%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 57170 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	224	1730	1076	308	340	6	0	0	0
1	B	220	1687	1053	298	330	6	0	0	0
1	G	228	1750	1088	312	344	6	0	0	0
1	H	217	1667	1041	293	327	6	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLU	-	expression tag	UNP C9QXI7
A	236	VAL	-	expression tag	UNP C9QXI7
A	237	LEU	-	expression tag	UNP C9QXI7
A	238	PHE	-	expression tag	UNP C9QXI7
A	239	GLN	-	expression tag	UNP C9QXI7
B	235	GLU	-	expression tag	UNP C9QXI7
B	236	VAL	-	expression tag	UNP C9QXI7
B	237	LEU	-	expression tag	UNP C9QXI7
B	238	PHE	-	expression tag	UNP C9QXI7
B	239	GLN	-	expression tag	UNP C9QXI7
G	235	GLU	-	expression tag	UNP C9QXI7
G	236	VAL	-	expression tag	UNP C9QXI7
G	237	LEU	-	expression tag	UNP C9QXI7
G	238	PHE	-	expression tag	UNP C9QXI7
G	239	GLN	-	expression tag	UNP C9QXI7
H	235	GLU	-	expression tag	UNP C9QXI7
H	236	VAL	-	expression tag	UNP C9QXI7
H	237	LEU	-	expression tag	UNP C9QXI7
H	238	PHE	-	expression tag	UNP C9QXI7
H	239	GLN	-	expression tag	UNP C9QXI7

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	1340	10570	6631	1841	2055	43	0	0	0
2	I	1340	10566	6629	1840	2054	43	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	1166	9107	5723	1634	1704	46	0	0	0
3	J	1334	10369	6513	1850	1957	49	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	89	691	421	129	140	1	0	0	0
4	K	79	627	382	118	126	1	0	0	0

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	542	4204	2625	752	801	26	0	0	0
5	L	539	4196	2619	749	802	26	0	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	D	1	1	1	0	0
6	J	1	1	1	0	0

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

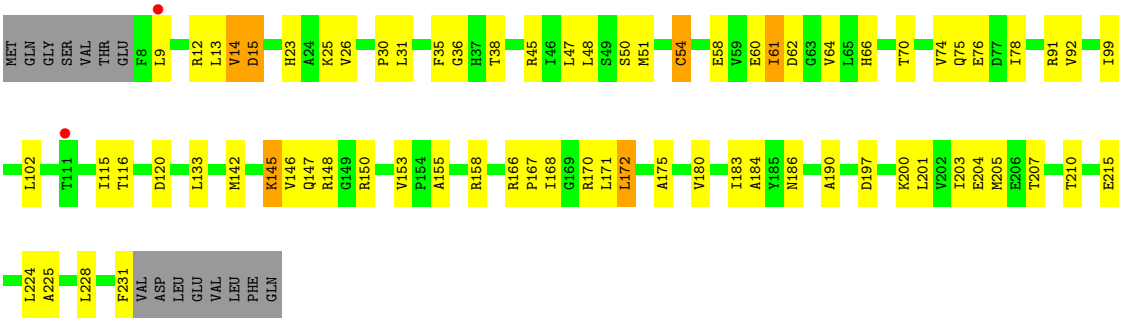
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
7	D	2	2	2	0	0
7	J	2	2	2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

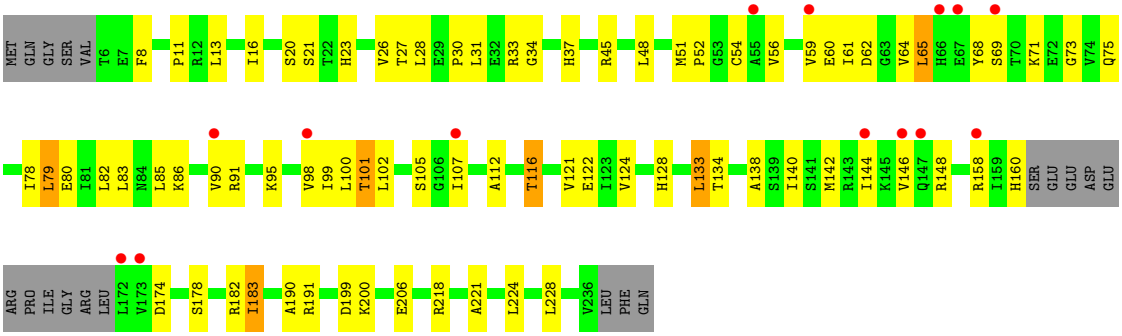
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



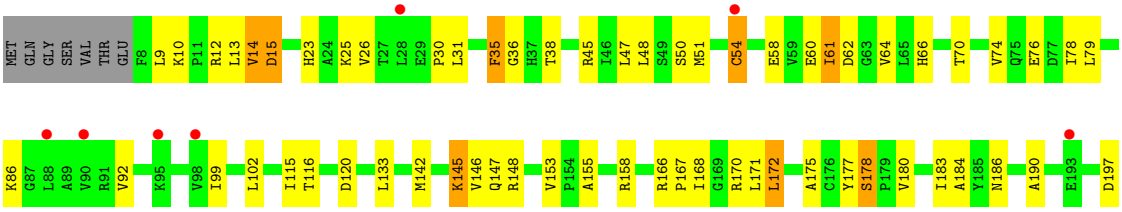
• Molecule 1: DNA-directed RNA polymerase subunit alpha

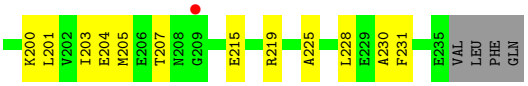
Chain B:



• Molecule 1: DNA-directed RNA polymerase subunit alpha

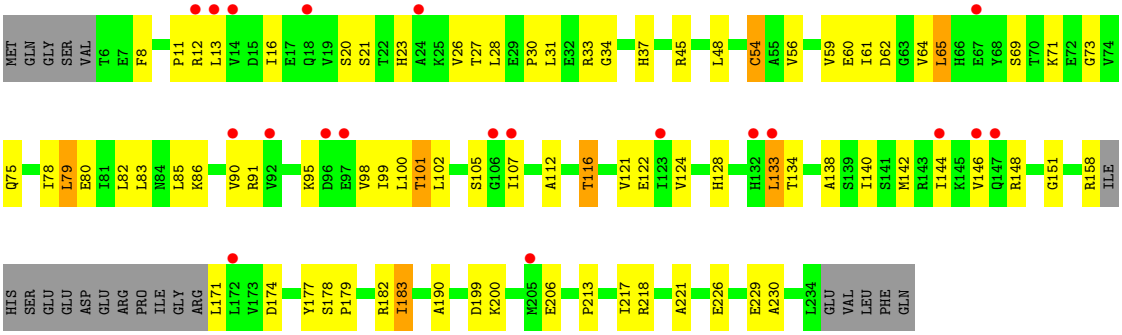
Chain G:





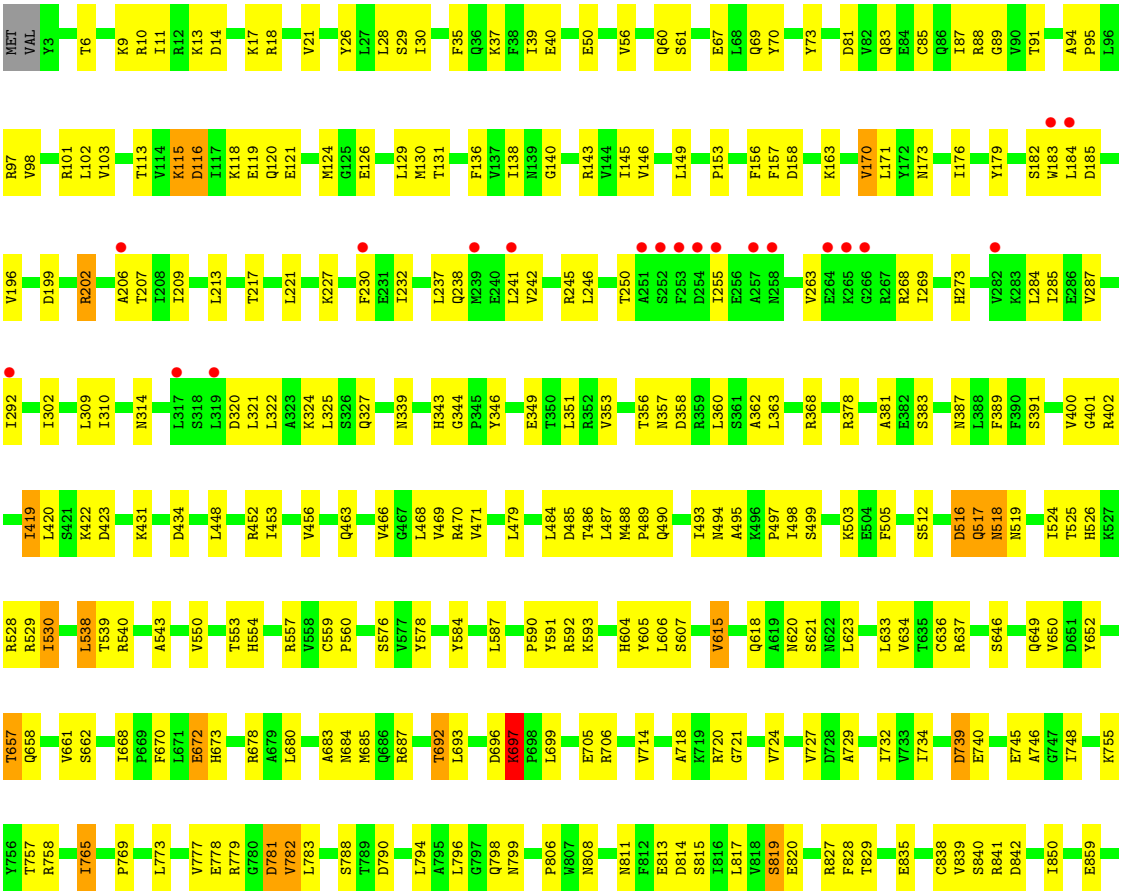
• Molecule 1: DNA-directed RNA polymerase subunit alpha

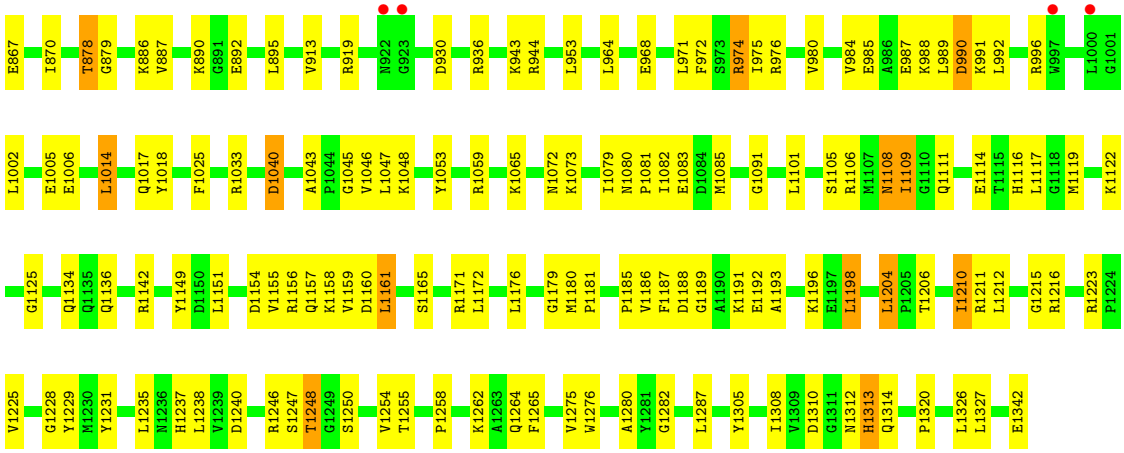
Chain H:



• Molecule 2: DNA-directed RNA polymerase subunit beta

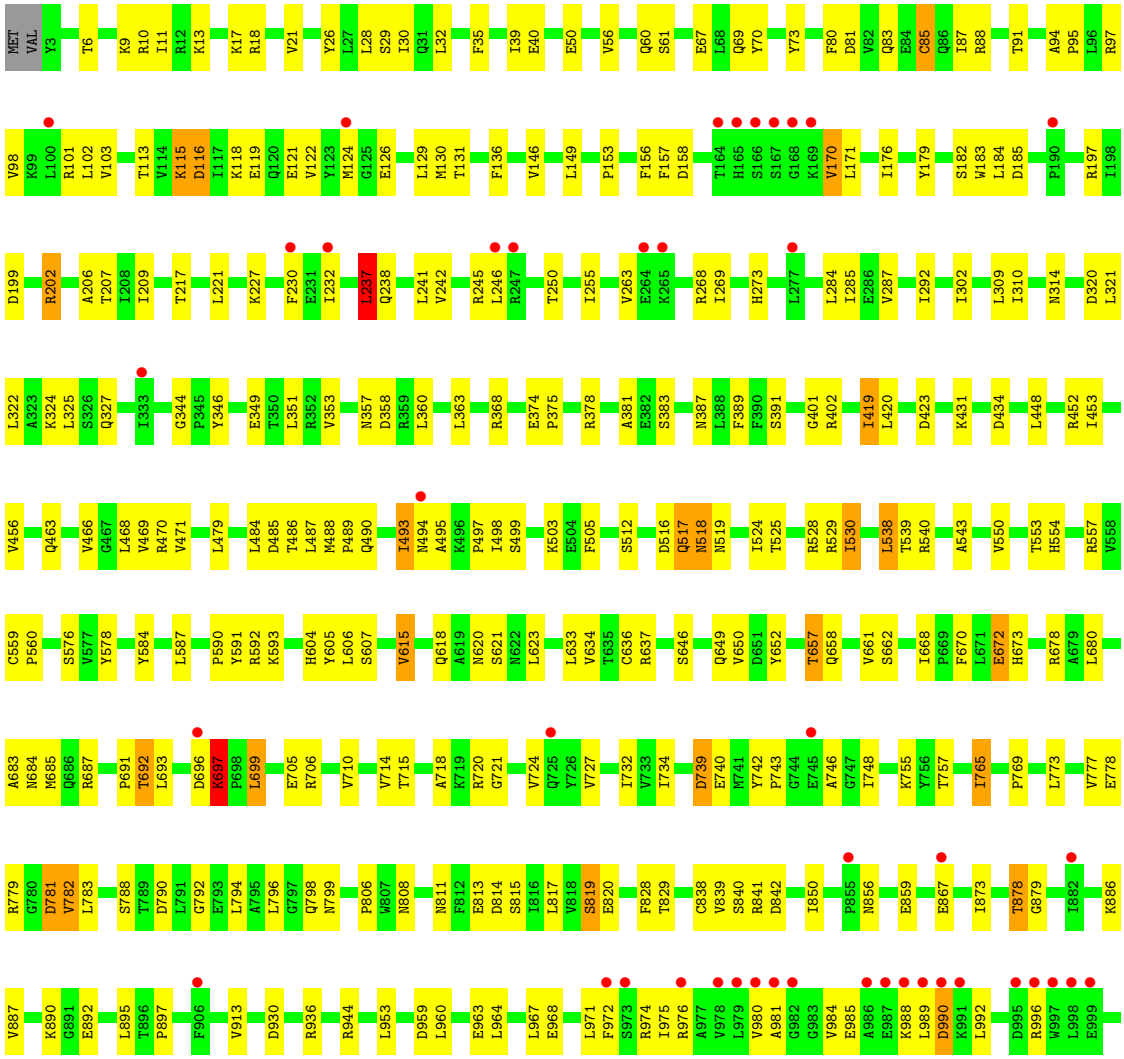
Chain C:

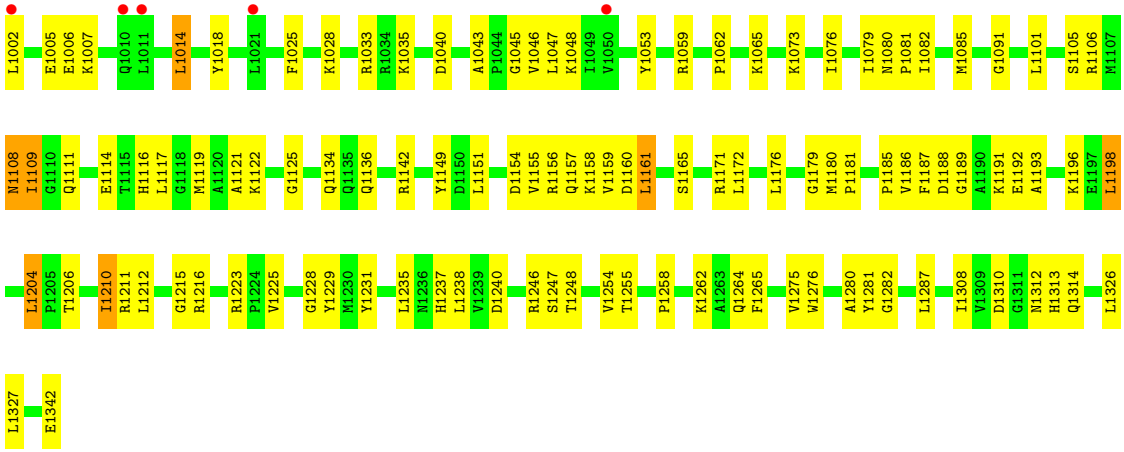




• Molecule 2: DNA-directed RNA polymerase subunit beta

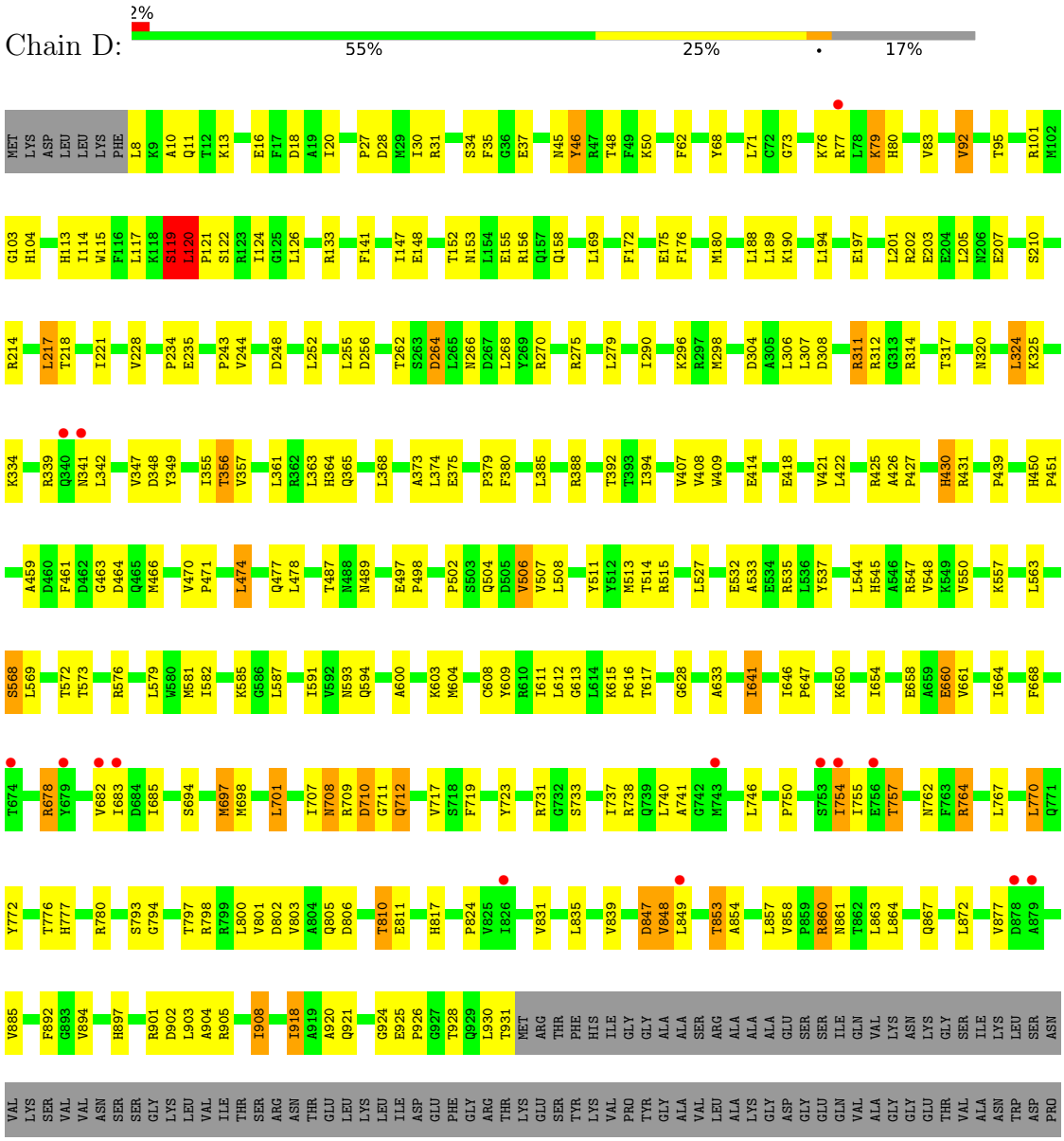
Chain I:

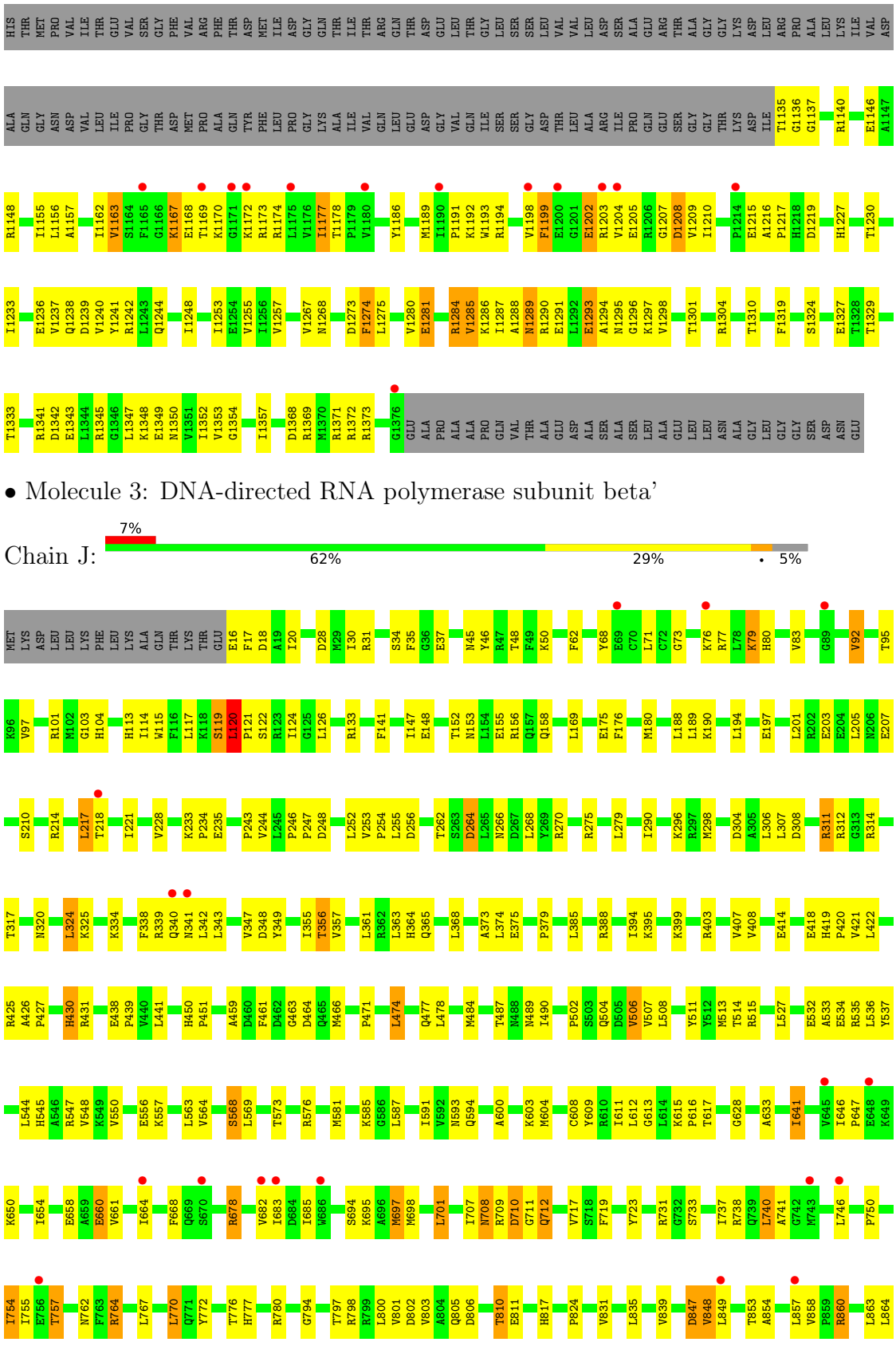




- Molecule 3: DNA-directed RNA polymerase subunit beta'

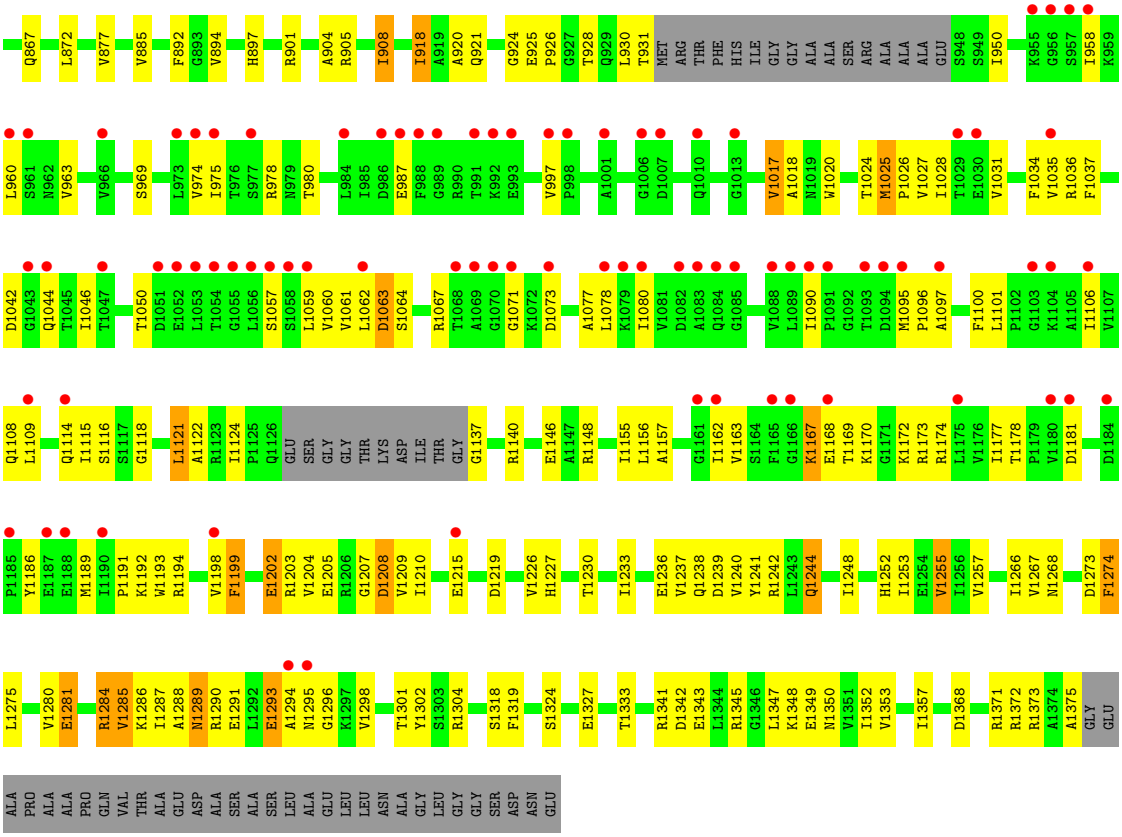
Chain D:





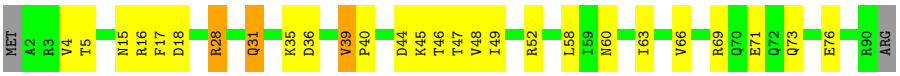
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain J:



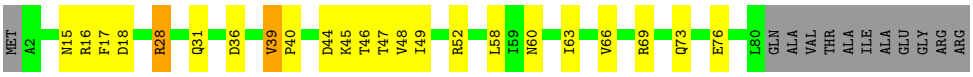
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



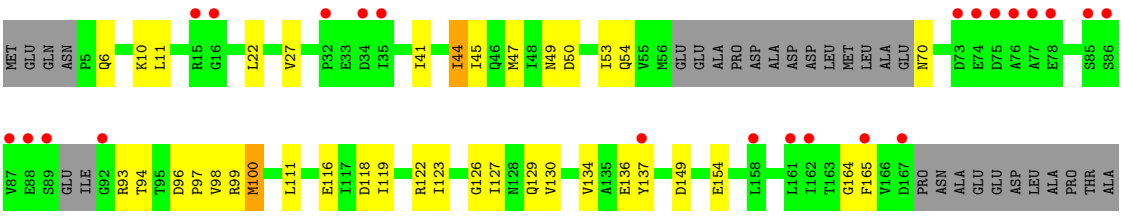
- Molecule 4: DNA-directed RNA polymerase subunit omega

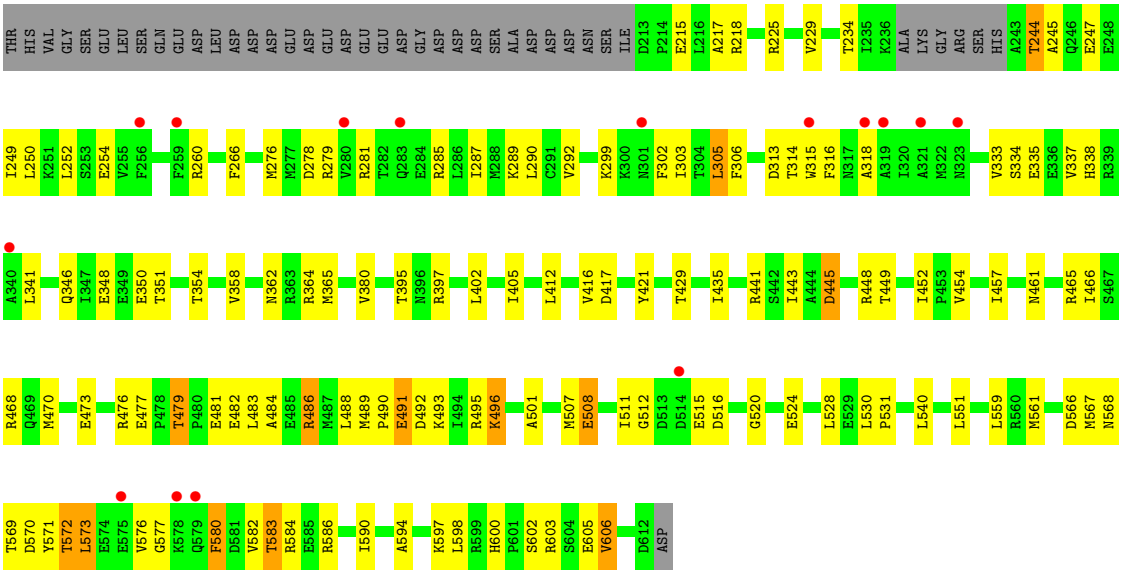
Chain K:



- Molecule 5: RNA polymerase sigma factor RpoD

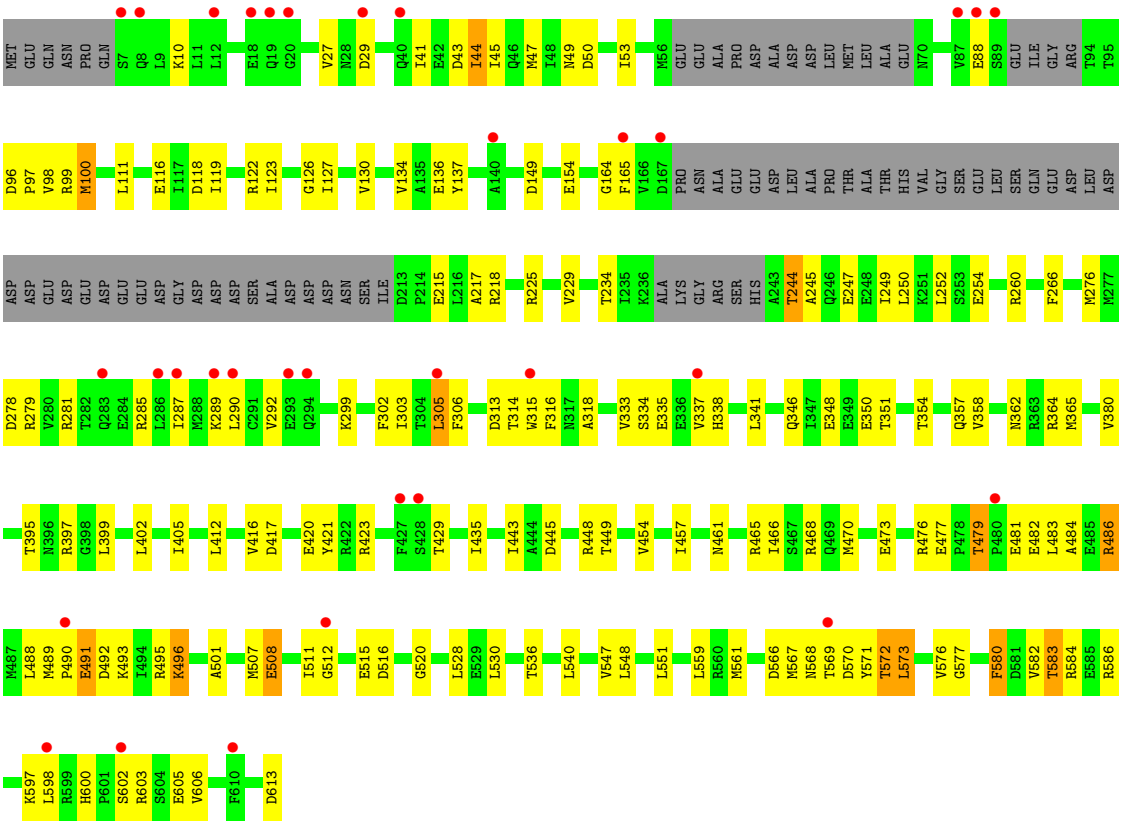
Chain F:





- Molecule 5: RNA polymerase sigma factor RpoD

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	186.68Å 206.39Å 308.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.78 – 3.84 44.78 – 3.84	Depositor EDS
% Data completeness (in resolution range)	98.2 (44.78-3.84) 98.3 (44.78-3.84)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 3.88Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.224 , 0.272 0.227 , 0.274	Depositor DCC
R_{free} test set	5631 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	142.8	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 63.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	57170	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.25	0/1751	0.51	0/2373
1	B	0.26	0/1707	0.49	0/2314
1	G	0.25	0/1771	0.53	0/2401
1	H	0.26	0/1686	0.49	0/2285
2	C	0.26	0/10739	0.48	1/14489 (0.0%)
2	I	0.26	0/10735	0.48	2/14484 (0.0%)
3	D	0.26	0/9246	0.48	1/12478 (0.0%)
3	J	0.26	0/10525	0.48	1/14212 (0.0%)
4	E	0.24	0/693	0.48	0/935
4	K	0.24	0/629	0.48	0/847
5	F	0.29	0/4254	0.51	2/5731 (0.0%)
5	L	0.29	0/4246	0.49	1/5720 (0.0%)
All	All	0.27	0/57982	0.49	8/78269 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
3	D	0	4
3	J	0	2
5	F	0	2
5	L	0	1
All	All	0	10

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	11	LEU	N-CA-C	-9.14	86.33	111.00
2	I	237	LEU	N-CA-C	5.38	125.53	111.00
3	D	120	LEU	N-CA-C	5.26	125.21	111.00
3	J	120	LEU	N-CA-C	5.25	125.18	111.00
2	C	516	ASP	CB-CG-OD2	5.23	123.01	118.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1161	LEU	Peptide
3	D	119	SER	Peptide,Mainchain
3	D	120	LEU	Peptide
3	D	1296	GLY	Peptide
5	F	6	GLN	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1730	0	1756	48	0
1	B	1687	0	1700	53	0
1	G	1750	0	1764	54	0
1	H	1667	0	1689	53	0
2	C	10570	0	10582	254	0
2	I	10566	0	10576	243	0
3	D	9107	0	9308	249	0
3	J	10369	0	10589	284	0
4	E	691	0	695	17	0
4	K	627	0	634	13	0
5	F	4204	0	4106	90	0
5	L	4196	0	4103	97	0
6	D	1	0	0	0	0
6	J	1	0	0	0	0
7	D	2	0	0	0	0
7	J	2	0	0	0	0
All	All	57170	0	57502	1328	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 1328 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.47	0.96
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.47	0.92
3:J:1044:GLN:HB3	3:J:1071:GLY:HA3	1.59	0.84
2:I:806:PRO:HA	2:I:811:ASN:HD21	1.42	0.84
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.43	0.84

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	222/239 (93%)	193 (87%)	27 (12%)	2 (1%)	17	53
1	B	216/239 (90%)	190 (88%)	26 (12%)	0	100	100
1	G	226/239 (95%)	196 (87%)	27 (12%)	3 (1%)	12	46
1	H	213/239 (89%)	190 (89%)	23 (11%)	0	100	100
2	C	1338/1342 (100%)	1233 (92%)	101 (8%)	4 (0%)	41	74
2	I	1338/1342 (100%)	1234 (92%)	99 (7%)	5 (0%)	34	70
3	D	1162/1407 (83%)	1061 (91%)	97 (8%)	4 (0%)	41	74
3	J	1328/1407 (94%)	1213 (91%)	111 (8%)	4 (0%)	41	74
4	E	87/91 (96%)	81 (93%)	6 (7%)	0	100	100
4	K	77/91 (85%)	73 (95%)	4 (5%)	0	100	100
5	F	532/613 (87%)	480 (90%)	52 (10%)	0	100	100
5	L	529/613 (86%)	480 (91%)	49 (9%)	0	100	100
All	All	7268/7862 (92%)	6624 (91%)	622 (9%)	22 (0%)	41	74

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	120	LEU
3	J	120	LEU
2	C	170	VAL
2	I	170	VAL
2	I	237	LEU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	191/206 (93%)	180 (94%)	11 (6%)	20	51
1	B	184/206 (89%)	168 (91%)	16 (9%)	10	38
1	G	191/206 (93%)	180 (94%)	11 (6%)	20	51
1	H	183/206 (89%)	168 (92%)	15 (8%)	11	40
2	C	1155/1157 (100%)	1063 (92%)	92 (8%)	12	41
2	I	1154/1157 (100%)	1063 (92%)	91 (8%)	12	42
3	D	975/1168 (84%)	883 (91%)	92 (9%)	8	34
3	J	1117/1168 (96%)	1015 (91%)	102 (9%)	9	36
4	E	72/75 (96%)	66 (92%)	6 (8%)	11	40
4	K	67/75 (89%)	61 (91%)	6 (9%)	9	36
5	F	426/540 (79%)	387 (91%)	39 (9%)	9	35
5	L	428/540 (79%)	391 (91%)	37 (9%)	10	39
All	All	6143/6704 (92%)	5625 (92%)	518 (8%)	11	40

5 of 518 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	1215	GLU
4	K	31	GLN
3	J	1209	VAL
3	D	1186	TYR

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Mol	Chain	Res	Type
3	D	1155	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	472	GLN
5	L	406	GLN
2	I	1111	GLN
3	J	419	HIS
2	I	1108	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	224/239 (93%)	-0.04	2 (0%)	84	78	57, 89, 134, 170	0
1	B	220/239 (92%)	0.19	14 (6%)	19	14	57, 121, 154, 165	0
1	G	228/239 (95%)	0.14	8 (3%)	44	36	84, 122, 155, 170	0
1	H	217/239 (90%)	0.35	20 (9%)	9	7	90, 134, 157, 166	0
2	C	1340/1342 (99%)	-0.07	24 (1%)	68	61	31, 86, 140, 175	0
2	I	1340/1342 (99%)	0.01	49 (3%)	41	33	41, 105, 151, 183	0
3	D	1166/1407 (82%)	-0.04	28 (2%)	59	50	28, 78, 140, 170	0
3	J	1334/1407 (94%)	0.25	102 (7%)	13	11	33, 99, 159, 185	0
4	E	89/91 (97%)	-0.25	0	100	100	38, 82, 122, 129	0
4	K	79/91 (86%)	-0.25	0	100	100	60, 96, 144, 154	0
5	F	542/613 (88%)	0.15	38 (7%)	16	12	49, 127, 166, 196	0
5	L	539/613 (87%)	0.06	33 (6%)	21	16	62, 125, 165, 179	0
All	All	7318/7862 (93%)	0.06	318 (4%)	35	29	28, 102, 155, 196	0

The worst 5 of 318 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	1054	THR	10.0
5	F	89	SER	8.3
5	L	7	SER	8.2
5	F	167	ASP	8.0
2	C	265	LYS	7.4

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	D	1501	1/1	0.85	0.51	72,72,72,72	0
6	MG	J	1501	1/1	0.85	0.63	74,74,74,74	0
7	ZN	D	1503	1/1	0.90	0.40	138,138,138,138	0
7	ZN	J	1502	1/1	0.94	0.13	107,107,107,107	0
7	ZN	D	1502	1/1	0.97	0.12	103,103,103,103	0
7	ZN	J	1503	1/1	0.99	0.18	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.